1-1-2012

Predicting the fate of emerging trace organic contaminants of concern during MBR treatment based on their molecular properties

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Abstract

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Keywords

molecular, during, mbr, treatment, properties, predicting, their, fate, emerging, trace, organic, contaminants, concern

Disciplines

Engineering | Science and Technology Studies

Publication Details

Wijekoon, K. C., Nghiem, L. D., Hai, F. I., Kang, J. & Price, W. E. (2012). Predicting the fate of emerging trace organic contaminants of concern during MBR treatment based on their molecular properties. Procedia Engineering, 44 (N/A), 980-982.

Title:

Predicting the fate of emerging trace organic contaminants of concern during MBR treatment based on their molecular properties

Authors & affiliations:

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We demonstrate that the fate of emerging trace organic contaminants during membrane bioreactor (MBR) treatment can be qualitatively predicted by assessing their molecular properties. This work further expands the qualitative framework for the prediction of trace organic removal by MBR treatment reported in our recent study [1]. A set of 30 emerging trace organic contaminants was selected for this investigation. The removal efficiency of some of these emerging trace organics by MBR have not been previously reported in the literature. Examples include phytoestrogens (such as enterolactone and formnonetine) and UV filters (such as benzophenone, oxybenzone, and octocrylene) which are frequently found at trace levels in natural water and raw sewage in Australia [2-3]. A laboratory scale MBR system was used in this study (Figure 1). The MBR system was equipped with an external ceramic membrane module (nominal pore size of 0.1 μm), a temperature control unit, a glass reactor (of 5 L in active volume), air pump, and influent and effluent pumps which were controlled by a personal computer. The MBR system was seeded with sludge obtained from the Wollongong Wastewater Treatment Plant in Wollongong, Australia. A synthetic wastewater was used in this study and the composition of this synthetic wastewater is available elsewhere [4]. After over 100 days of acclimatisation, trace organic contaminants were continuously introduced into the synthetic wastewater at concentration of approximately 5 μg/L of each compound. The MBR system was operated under a constant condition with the hydraulic retention time, temperature, dissolved oxygen concentration, and mixed liquor pH of 26 h, 25.8 ± 0.3 ºC, 2.3 ± 0.3 mg/L, and 7.2 ± 0.3, respectively. The mixed liquor suspended solid concentration in the reactor was maintained at 5.0 ± 0.5 g/L by withdrawing the excess sludge every 3 – 4 days, resulting in a sludge retention time of approximately 88 days.

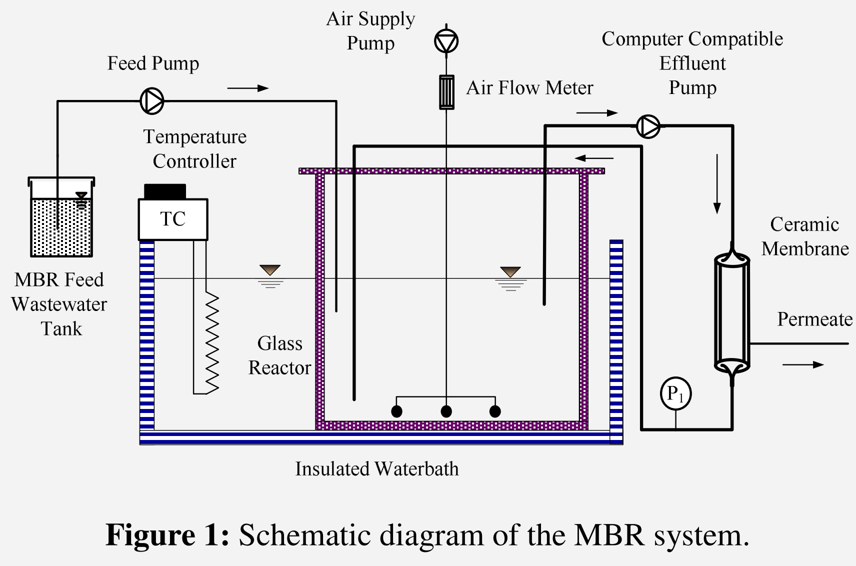

Figure 1: Schematic diagram of the MBR system.

Concentration of trace organics in the aqueous phase were determined using a previously developed method involving solid phase extraction (SPE) followed by GC/MS quantification [4]. An ultrasonication solvent extraction technique was used to extract the trace organics from the sludge. Sludge samples were first centrifuged and the solid pellet was freeze dried at – 53 ºC and 0.02 mbar using an Alpha 1-2 LD Plus freeze dryer. The dried sludge was grounded into powder prior to the solvent extraction process. The extracted analysts were then diluted with MilliQ water and were analysed using the same SPE-GC/MS analytical method used the aqueous samples as described above. All analyses were conducted in duplicate.

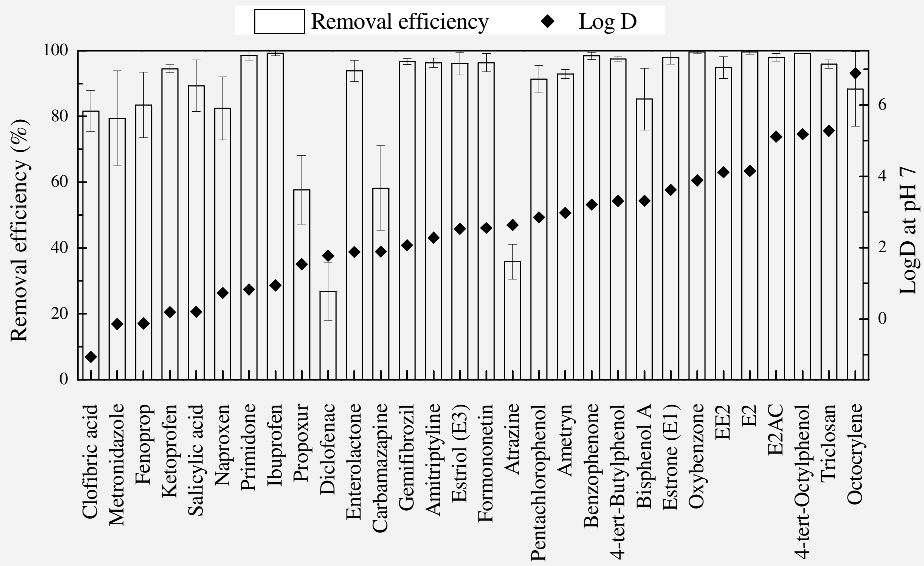

Figure 2: Trace organic removal by the MBR system under stable operating conditions; The error bars represent the standard deviation of repetitive measurements taken consecutively one a week over 6 weeks.

Results reported here highlight hydrophobicity as a major factor governing the removal of trace organics from the aqueous phase. The removal efficiencies of all 11 very hydrophobic trace organics (i.e., Log D at pH 7 > 3) selected in this study consistently showed high removal efficiencies of 80% or above (Figure 2). Of the 30 compounds selected in this study, four (i.e., propoxur, diclofenac, carbamazepine, and atrazine) showed removal efficiencies of approximately 50% or below. These low removal efficiencies can be attributed to their low hydrophobicity and more importantly the occurrence of strong electron withdrawing functional groups (EWGs) such as chlorine and amide in their molecular structure as previously delineated by Tadkaew et al., [1]. Results reported in this study also show that the fate of trace organic contaminants is also governed by their molecular properties. The concentration of trace organics in the sludge phase increased after they had been introduced into the synthetic wastewater only if they contain EWGs in the molecular structure or/and are hydrophobic. In fact, the concentrations of all 10 compounds with log D at pH 7 of above 3 in the sludge phase were negligible because they do not have EWGs in their molecular structure and thus are readily biodegradable. On the other hand, the average concentration of triclosan in the sludge was 1278 ng/g and was the highest of all compounds investigated in this study. The high concentration of triclosan in the sludge can be explained by its very high log D value (of 5.28 at pH 7) and the presence of a strong EWG (i.e. chlorine) in its molecular structure which renders the compound very persistent to biological degradation. The concentration of triclosan (and other compounds) in the sludge was relatively constant over the 6 weeks duration of this study and this can be attributed to the regular removal of excess sludge. It is noteworthy that a mass balance calculation reveals that biodegradation accounts for 54.5% of the fate of triclosan during MBR treatment (Figure 3). In comparison, the concentrations of propoxur, diclofenac, carbamazepine, and atrazine (which are not very hydrophobic and have shown low removal efficiency from the aqueous phase) in the sludge were considerably smaller than that of triclosan and the biodegradation only accounts for a small fraction of the fate of these compounds during MBR treatment (Figure 3). Results reported in Figure 3 provide evidence of the enhanced biodegradation phenomenon when trace organics can adsorb into the sludge and subsequently be biodegraded. In addition, results reported here suggest that the fate of trace organics in both the aqueous and sludge phases can be predicted by assessing the presence of EWGs in their molecular structure and their hydrophobicity.

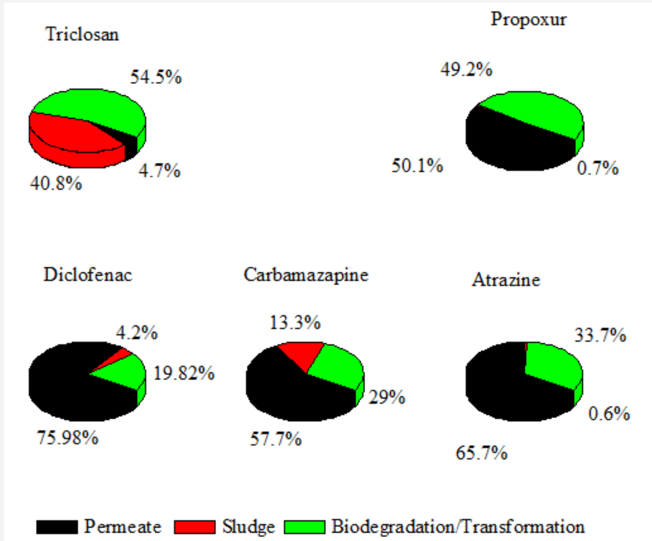

Figure 3: Fate of trace organics with strong electron withdrawing functional groups during MBR treatment.

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